Amendments to the Claims

This listing of claims will replace all prior versions, and listing of claims, in the application:

1. (currently amended) A computer-implemented method for use in deriving a chemical structure diagram, comprising:

identifying, from a connection table for a chemical structure, an instance of chemical structural symmetry in the chemical structure;

wherein the instance of symmetry includes symmetrically equivalent atoms and bonds;

laying out symmetrically equivalent atoms and bonds in the chemical structure diagram ~~in accordance with~~ to express the identified symmetry; and

outputting a representation of the chemical structure.

2-5. (canceled)

6-8. (canceled)

9. (currently amended) ~~Computer software, residing on a~~ A computer-readable storage medium encoded with~~, comprising~~ a set of instructions for use in a computer system to ~~help~~ cause the computer system to derive a chemical structure diagram, the instructions causing the system to:

identify, from a connection table for a chemical structure, an instance of chemical structural symmetry in the chemical structure, wherein the instance of chemical structural symmetry includes symmetrically equivalent atoms and bonds; and

lay out symmetrically equivalent atoms and bonds in the chemical structure diagram ~~in accordance with~~ to express the identified symmetry; and

output a representation of the chemical structure.

10-12. (canceled)

13. (previously presented) The method of claim 1, wherein the instance of chemical structural symmetry is based on rotational symmetry.

14. (previously presented) The method of claim 1, wherein the instance of chemical structural symmetry is based on reflective symmetry.

15. (previously presented) The method of claim 1, wherein the instance of chemical structural symmetry is based on inversive symmetry.

16. (previously presented) The method of claim 1, further comprising:

basing the identification on stereochemistry.

17. (previously presented) The method of claim 1, further comprising:

basing the identification on rotational symmetry, reflective symmetry, and stereochemistry.

18. (previously presented) The method of claim 1, further comprising:

basing the identification on double bond stereochemistry.

19. (previously presented) The method of claim 1, further comprising:

determining a pivot point for the list.

20. (previously presented) The method of claim 1, further comprising:

determining a graph-theoretic center for the list.

21. (previously presented) The method of claim 1, further comprising:

determining a symmetric order for the instance of chemical structural symmetry.

22. (previously presented) The method of claim 1, further comprising:

determining whether an atom belongs to the identified instance of chemical structural symmetry.

23. (previously presented) The method of claim 1, further comprising:

determining whether a bond belongs to the identified instance of chemical structural symmetry.

24. (previously presented) The method of claim 1, further comprising:

in the event the identified instance of chemical structural symmetry is reflective, selecting a position on an opposite side of a mirror line.

25. (previously presented) The method of claim 1, further comprising:

in the event the identified instance of chemical structural symmetry is rotative, selecting a position based on a pivot point.

26. (previously presented) The method of claim 1, further comprising:

rotating the chemical structure diagram so that a mirror plane in the chemical structure diagram is horizontal.

27. (previously presented) The method of claim 1, further comprising:

rotating the chemical structure diagram so that a mirror plane in the chemical structure diagram is vertical.

28. (currently amended) A computer-implemented method for use in deriving a chemical structure diagram, comprising:

identifying an instance of chemical structural symmetry in the chemical structure;

wherein the instance of symmetry includes symmetrically equivalent atoms and bonds;

laying out symmetrically equivalent atoms and bonds in the chemical structure diagram ~~in accordance with~~ to express the identified symmetry; and

outputting a representation of the chemical structure.

29. (previously presented) The method of claim 28, wherein the instance of chemical structural symmetry is based on rotational symmetry.

30. (previously presented) The method of claim 28, wherein the instance of chemical structural symmetry is based on reflective symmetry.

31. (previously presented) The method of claim 28, wherein the instance of chemical structural symmetry is based on inversive symmetry.

32. (previously presented) The method of claim 28, further comprising:

basing the identification on stereochemistry.

33. (previously presented) The method of claim 28, further comprising:

basing the identification on rotational symmetry, reflective symmetry, and stereochemistry.

34. (previously presented) The method of claim 28, further comprising:

basing the identification on double bond stereochemistry.

35. (currently amended) A ~~system~~ computer-readable storage medium encoded with a set of instructions to cause a system ~~for use in deriving~~ to derive a chemical structure diagram, the instructions causing the system to ~~comprising~~:

~~an identifier~~ identify~~ing~~ an instance of chemical structural symmetry in the chemical structure, wherein the instance of symmetry includes symmetrically equivalent atoms and bonds;

~~a positioner~~ lay~~ing~~ out symmetrically equivalent atoms and bonds in the chemical structure diagram ~~in accordance with~~ to express the identified symmetry; and

~~an output device~~ output~~ting~~ a representation of the chemical structure.